Anekant Education Society's

Tuljaram Chaturchand College

of Arts, Science, Commerce, Baramati

(Autonomous)

DEPARTMENT OF CHEMISTRY

(Faculty of Science and Technology)

Two Year MSc Degree Program Chemistry

MSc Organic Chemistry

(2022 Pattern)

Choice Based Credit System Structure and Syllabus

(To be implemented from June 2022)

M. Sc. - II Organic Chemistry

Semester–III

PSCH0 231: Designing of organic synthesis and Heterocyclic Chemistry

(48L+12 T) (4 Credit)

Course Objective: On completion of the course, the student will be able to:

1) To provide students with a solid foundation in the principles and concepts of heterocyclic chemistry, including the classification, nomenclature, and synthesis of heterocyclic compounds.
2) To explore the reactivity patterns of different heterocyclic systems and their synthetic methods, including both traditional and modern approaches.
3) To enhance students' problem-solving skills and critical thinking abilities by providing them with opportunities to analyze and solve complex problems related to heterocyclic chemistry.
4) To provide students with a thorough understanding of the principles and strategies involved in retrosynthetic analysis, including the identification of key functional groups, disconnections, and the selection of appropriate synthetic pathways.
5) To introduce students to the concept of protecting functional groups during organic synthesis and the selection of appropriate protective groups.
6) To understand the rationale behind protection, the methods for introducing and removing protective groups, and the impact of protective groups on reaction selectivity.
7) To develop students' problem-solving skills and critical thinking abilities by providing them with opportunities to analyze complex synthetic problems, propose synthetic routes, and evaluate the feasibility and efficiency of different strategies.

Course Outcomes : On completion of the course, the student should be able to:

CO1. Get the knowledge of designing the new molecule and heterocyclic compound synthesis.

CO2. Expertise in reactions using protection and deprotection methods.

CO3. Demonstrate the skill of critical thinking for retrosynthesis of largest molecule and can able to synthesize them by designing simple organic methodology.

CO4. Describe methods for synthesis and transformation of the most common functional groups

CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.

CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis.

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

1. Designing of organic synthesis **(24 L)**

Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions as illustrated in the synthesis of polypeptide and polynucleotide, enamines, An introduction to Synthons and synthetic equivalents, disconnecttion approach, functional group interconversions. Importance of the Order of events in organic synthesis, Chemoselectivity, Regioselectivity. Umpolung in organic synthesis, FGI, divergent vs. convergent syntheses. Synthesis of some typical organic molecules-Abscisic acid, Longifolene Ref. 1-9

2.Heterocyclic Chemistry **(24 L)**

a) Five and six membered heterocycles with one and two heteroatoms:
   Synthesis, reactivity, aromatic character and importance of following heterocyclic compounds: Furan, Pyrrole, Thiophene, Pyrazole, Imidazole, Pyridine
b) Synthesis, reactivity, aromatic character and importance of following heterocyclic compounds: Condensed five and six membered heterocycles: Benzofuran, Indole, Quinoline
c) Condensed five membered heterocycles: Benzoxazole, Benzthiazole, Benzimidazole
d) Synthesis of ranitidine, papavarine, amlodipine, bromouridine, tryptophan, thiamine, chloroquine Ref.10-17

References:

1. Heterocyclic Chemistry- R.K. Bansal
2. Designing of organic synthesis– S.Warren (Wiley)
3. Some modern methods of organic synthesis–W.Carruthers (Cambridge)
4. Organic chemistry–J. Clayden, N. Greeves, S.Warren andP. Wothers (OxfordPress)
5. Advanced organic chemistry,PartB–F.ACareyandR.J.Sundberg,5thedition(2007)
6. Guide book to organic synthesis-RKMeckie,D MSmithand RAAtken
7. Organic synthesis-RobertE Ireland
8. Strategic Applications of named reactions in organicsynthesis-LaszloKurtiandBarbaraCzako
9. Organic synthesisthroughdisconnectionapproach-P.S. Kalsi
10. Heterocyclic Chemistry-T. Gilchrist
11. Anintroduction to the chemistryofheterocyclic compounds-R M Acheso
12. HeterocyclicChemistry-JAJoule andK Mills
13. Principlesofmodernheterocyclicchemistry-APaquette
14. Theessenceof Heterocyclic Chemistry- A. R.Parikh, Hansa Parikh, Ranjan Khunt
15. HandbookofHeterocyclic Chemistry- ARKatritzky,AFPozharskii
16. HeterocyclicChemistry-II-R.R.Gupta,M Kumar,V Gupta,Springer(India)pvt

Choice Based Credit System Syllabus
(2022 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III) **Subject**:Organic Chemistry
Course: Designing of org. synthesis and Heterocyclic Chemistry **Course Code**: PSCHO-231
Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Program Outcomes (POs) and Course Outcomes (COs) Matrix with Weightage:

	Programme Outcomes(POs)								
Course Outcomes	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**
CO1	3	0	0	0	0	3	0	0	2
CO2	2	2	0	3	0	0	0	0	0
CO3	1	3	0	0	0	0	0	0	0
CO4	2	0	0	2	3	0	0	0	0
CO5	1	3	0	2	2	0	0	0	0
CO6	3	3	0	0	0	3	0	0	2
CO7	0	0	0	2	2	0	3	0	3

Justification for the mapping

PO1 (Disciplinary Knowledge):
CO1. Get the knowledge of designing the new molecule and heterocyclic compound synthesis.
CO2. Expertise in reactions using protection and deprotection methods.
CO3. demonstrate the skill of critical thinking for retrosynthesis of largest molecule and can able to synthesize them by designing simple organic methodology.
CO4. Describe methods for synthesis and transformation of the most common functional groups
CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.
CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis.

PO2 (Critical Thinking and Problem Solving):
CO2. Expertise in reactions using protection and deprotection methods.
CO3 demonstrate the skill of critical thinking for retrosynthesis of largest molecule and can able to synthesize them by designing simple organic methodology.
CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.
CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis.

PO4 (Research-related Skills and Scientific Temper):
CO2. Expertise in reactions using protection and deprotection methods.
CO4. Describe methods for synthesis and transformation of the most common functional groups.
CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.
CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

PO5 (Trans-disciplinary Knowledge):

CO4. Describe methods for synthesis and transformation of the most common functional groups.

CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

PO6 (Personal and Professional Competence):

CO1 Get the knowledge of designing the new molecule and heterocyclic compound synthesis.

CO 6 Apply the knowledge of organometallic reagents and reactions in organic synthesis

PO7 (Effective Citizenship and Ethics):

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

PO9 (Self-directed and Life-long Learning):

CO1. Get the knowledge of designing the new molecule and heterocyclic compound synthesis

CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

PSCHO-232: Spectroscopic Methods in Structure Determination
(48L+12 T)(4 Credit)

Course Objective:

1) Students will learn the fundamental principles and theory behind NMR, IR, and Mass Spectroscopy techniques.
2) Students will develop the skills to interpret NMR, IR, and Mass Spectroscopy spectra, including identifying functional groups, determining chemical shifts, analyzing peak patterns, and understanding fragmentation patterns in Mass Spectroscopy.
3) Students will gain knowledge about the instrumentation used in NMR, IR, and Mass Spectroscopy, including the components and operation of the instruments.
4) Students will also learn data analysis techniques, such as peak integration and spectral manipulation.
5) Students will learn how to use NMR, IR, and Mass Spectroscopy data to determine the structure of organic compounds.
6) Students will assign peaks in NMR spectra, correlating NMR data with molecular structure, and using IR and Mass Spectroscopy data to support structural assignments.
7) Students will explore the various applications of NMR, IR, and Mass Spectroscopy in chemistry, such as identifying unknown compounds, monitoring chemical reactions, and studying molecular dynamics.

Course Outcomes : On completion of the course, the student should be able to:

CO1. Understand the principles and theory behind different spectroscopic methods.

CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.

CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.

CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.

CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.

CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.

CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis.

^{1}H NMR Spectroscopy **(14L)**

Recapitulation of basic principle, Chemical shift, factors influencing chemical shift, deshielding, chemical shift values and correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and other nuclei(alcohols, phenols, enols, acids, amides and mercaptans), chemical exchange, effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four andfive nuclei (first order spectra), factors effecting coupling constant "*J*", Spin decoupling.

Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear over-hauser effect (NOE), and resonance of other nuclei like ^{31}P

^{13}CNMR spectroscopy **(8 L)**

FT NMR, Types of ^{13}C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, , DEPT with 3 different angles, chemical shift, calculations of chemical shifts ofaliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affectingchemical shifts, chemical shifts of solvents, Homo nuclear (^{13}C-^{13}C) and Hetero nuclear (^{13}C-^{1}H)coupling constants.

2D NMR Techniques **(6L)**

General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)-Homo COSY (^{1}H-^{1}H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications. Illustrative example of COSY, HSQC in carbohydrate characterization.

Mass Spectrometry **(10L)**

Instrumentation, various methods of ionization (fieldionization, field desorption, SIMS, FAB, MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrapole mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors controlling fragmentation

Problems based onjointapplication of UV,IR,PMR,CMR, and Mass. **(10 L)**

(Includingreactionsequences)

References:

1. IntroductiontoSpectroscopy-D.L.Pavia,G.M.Lampman,G.S.Kriz,3rdEd.(Harcourtcollege publishers).
2. SpectrometricidentificationoforganiccompoundsR.M.Silverstein,F.X.Webster,6th Ed.

JohnWileyand Sons.
3. Spectroscopicmethodsinorganicchemistry-D.H.WilliamsandI.FlemmingMcGrawHill
4. Absorption spectroscopyoforganic molecules - V. M. Parikh
5. NuclearMagneticResonance-BasicPrinciples-Atta-Ur-Rehman,Springer-Verlag(1986).
6. Oneand Two dimensional NMR Spectroscopy-Atta-Ur-Rehman, Elsevier(1989).
7. OrganicstructureAnalysis-PhillipCrews,Rodriguez,Jaspars,OxfordUniversityPress (1998)
8. OrganicstructuralSpectroscopy-JosephB.Lambert,Shurvell,Lightner,Cooks,Prentice-Hall(1998).
9. Organicstructuresfromspectra-FieldL.D.,KalmanJ.R.andSternhellS.4thEd.JohnWileyandsonsLtd.
10. Spectroscopicidentificationoforganiccompound-R.M.Silverstein,G.C.Basslerand T.C.Morril,JohnWiley
11. Introductionto NMRspectroscopy-R. J.Abrahm,J. Fisherand P. loftusWiley
12. Organicspectroscopy-Williamkemp,E. L.B. withMcMillan
13. Spectroscopyoforganicmolecule-P.S.Kalsi,Wiley,Esterna,New Delhi
14. Organicspectroscopy-R.T.MorrisonandR.N.Boyd
15. PracticalNMR spectroscopy-M.L. Martin,J.J. Delpench,andD.J. Martyin
16. Spectroscopicmethodsin organicchemistry-D.H. Willson,I.Fleming
17. Spectroscopyinorganicchemistry- C.N. R.RaoandJ.R. Ferraro
18. NMR–Basicprinciple andapplication-H.Guntur
19. InterpretationofNMR spectra-RoyH.Bible
20. CarbohydrateCharacterizationthroughMultidimensionalNMR:AnUndergraduateOrganicLaboratoryExperiment.*J. Chem.Educ.***2020**, 97(1),195-199
21. Mass spectrometryorganicchemicalapplications-JH Banyon

Choice Based Credit System Syllabus
(2022 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III) **Subject**:Organic Chemistry
Course: Spectroscopic Methods in Structure Determination **Course Code**: PSCHO-232
Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	2	0	1	0	0	0
CO2	2	3	0	0	0	2	0	0	0
CO3	3	3	0	0	2	0	0	0	0
CO4	1	0	0	3	0	2	0	0	0
CO5	1	2	0	2	3	0	0	0	0
CO6	3	0	0	2	0	3	0	0	2
CO7	1	3	0	0	0	2	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):
CO1. Understand the principles and theory behind different spectroscopic methods.
CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.
CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.
CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.
CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.
CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.
CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis

PO2 (Critical Thinking and Problem Solving)
CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.
CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.
CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.
CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis

PO4 (Research-related Skills and Scientific Temper):
CO1. Understand the principles and theory behind different spectroscopic methods.
CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.
CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.

CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.

PO5 (Trans-disciplinary Knowledge):
CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.
CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.

PO6 (Personal and Professional Competence):
CO1. Understand the principles and theory behind different spectroscopic methods.
CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.
CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.
CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.
CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis

PO9 (Self-directed and Life-long Learning):
CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.

PSCHO-233:Organic Stereochemistry-I and Organic Reaction Mechanism (48L+12 T)(4Credit)

Course Objective:

1) To explore the different conformations and their energy profiles of six-membered and fused bridge cage ring compounds. This includes understanding the factors that influence conformational stability and the interconversion between different conformers.
2) To study the stereochemistry of reactions involving six-membered and fused bridge cage ring compounds.
3) To gain a deep understanding of the stereochemistry of six-membered and fused bridge cage ring compounds, enabling them to analyze and predict stereochemical outcomes in reactions, design synthetic routes.
4) To explore the reactivity patterns and synthetic methods involving carbanions, including their generation, stability, and reactions with electrophiles. This includes understanding the factors that influence carbanion stability and the use of carbanions in carbon-carbon bond formation.
5) To examine the concept of neighboring group participation, which involves the influence of adjacent functional groups on the reactivity and selectivity of reactions..
6) To understand the principles and mechanisms of various types of neighboring group participation, such as anchimeric assistance and neighboring group assistance
7) To study the formation, reactivity, and synthetic applications of enamines, which are versatile intermediates in organic synthesis.

Course Outcomes : On completion of the course, the student should be able to;

CO1. Understand the principles of stereochemistry and apply them to analyze the stereochemistry of six-membered rings, rings other than six-membered, fused bridged, and caged rings.

CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions

CO3. Explain the formation and applications of enamines in organic synthesis.

CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.

CO5. Discuss the synthesis and reactions of carbenes and nitrenes in organic chemistry.

CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.

CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

Organic Stereochemistry-I **(24L)**

1. Stereochemistry of six membered rings. Ref.1,3, 4, 5

2. Stereochemistry of rings other than six membered Ref.1,3, 4, 5

3. Fused Bridged and caged rings Ref. 1,2, 3,4

Organic Reaction Mechanism

1. Carbanions: Formation, geometry,stability and related reactions- Aldol, α- halogenation, haloform reaction, Michael reaction, Robinson annulations, Mannich, Stobbe, Cannizaro's, Darzons, Dieckmann, Knoevegel, Benzoin, Perkin, Benzoin condensation, Grignard, Claisen condensation, Baylis-Hilman, Appel reaction, Corey-Fuchs reaction
Ref.6,7,8,10 **[12 L]**

2. Enamines:formation and applications of enamine in organic synthesis.Ref.9 **[4 L]**

3. NGP:Neighbouring group participation Ref.6 **[4 L]**

4. Synthesis and reactions of carbenes and nitrenes Ref.9 **[4 L]**

References:

1. Stereochemistry of carbon compounds - E.L. Eliel
2. Stereochemistry of carbon compounds - E.L.Eliel and S. H. Wilen
3. Stereochemistry of organic compounds –Nasipuri
4. Stereochemistry of organic compounds-Kalsi
5. Organic stereochemistry–Jagdamba Singh
6. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart andWinston)
7. Advanced organicchemistrybyJ. March, 6th Ed.
8. Advanced organic chemistry. F. A. Carey and R. J. Sundberg, Part A 5th Ed. Springer(2007)
9. Advanced organic chemistry. F. A. Carey and R. J. Sundberg, Part B 5th Ed.Springer(2007)
10. Organic Chemistry–J.Clayden,N. Greeves,S.WarrenandP. Wothers

Choice Based Credit System Syllabus
(2022 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III) **Subject**:Organic Chemistry
Course: Org. Stereochemistry-I and Org. Reaction Mechanism **Course Code**: PSCHO-233
Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	0	0	3	0	0	0
CO2	3	3	0	2	0	2	0	0	0
CO3	1	0	0	0	3	0	0	0	0
CO4	3	3	0	2	0	2	0	0	0
CO5	3	0	0	0	3	3	0	0	0
CO6	2	3	0	0	0	3	0	0	2
CO7	1	3	0	2	0	2	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):

CO1. Understand the principles of stereochemistry and apply them to analyze the stereochemistry of six-membered rings, rings other than six-membered, fused bridged, and caged rings.
CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions
CO3. Explain the formation and applications of enamines in organic synthesis.
CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.
CO5. Discuss the synthesis and reactions of carbenes and nitrenes in organic chemistry.
CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.
CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO2 (Critical Thinking and Problem Solving):

CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions.
CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.
CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.
CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO4 (Research-related Skills and Scientific Temper):

CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions
CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.
CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO5 (Trans-disciplinary Knowledge):
CO3. Explain the formation and applications of enamines in organic synthesis.
CO5. Discuss the synthesis and reactions of carbenes and nitrenes in organic chemistry.

PO6 (Personal and Professional Competence):
CO1. Understand the principles of stereochemistry and apply them to analyze the stereochemistry of six-membered rings, rings other than six-membered, fused bridged, and caged rings.
CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions
CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.
CO5. Discuss the synthesis and reactions of carbenes and nitrenes in organic chemistry.
CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.
CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO9 (Self-directed and Life-long Learning):
CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.

PSCHO -234:Photochemistry, Free radicals and Pericyclic Reactions

(48L+12 T)(4Credit)

Course Objective:

1) Students will develop a solid understanding of the theoretical principles and concepts that govern pericyclic reactions, including orbital symmetry, frontier molecular orbital theory, and the Woodward-Hoffmann rules.
2) Students will learn to recognize and differentiate between various types of pericyclic reactions, such as cycloadditions, electrocyclic reactions, sigmatropic rearrangements.
3) Students will learn to analyze and interpret the mechanisms of pericyclic reactions using molecular orbital theory
4) Students will explore the synthetic applications of pericyclic reactions, including their use in the construction of complex organic molecules and the synthesis of natural products.
5) Students will learn about the nature, properties, and reactivity of free radicals in organic chemistry.
6) Students will learn how to analyze and interpret the mechanisms of free radical reactions, including the initiation, propagation, and termination steps.
7) To provide students with a comprehensive understanding of the fundamental principles underlying photochemical reactions in organic chemistry. This includes the concepts of electronic excitation, energy transfer, and photochemical reactions involving singlet and triplet excited states.

Course Outcomes : On completion of the course, the student should be able to;

CO1. Understand the principles and mechanisms of photochemical reactions, including photo rearrangements, photo reduction, and photo oxidation.

CO2. Apply the concepts of photochemistry to analyze and predict the outcomes of photo substitution reactions, such as the Barton reaction.

CO3. Utilize photochemical reactions in synthesis, specifically the Isocomene synthesis.

CO4. Describe the characteristics and reactions of free radicals, including free radical substitution and addition to multiple bonds.

CO5. Apply free radicals in various synthetic reactions, such as the Hunsdiecker reaction and Barton Nitrite Photolysis reaction.

CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.

CO7. Explain the chemistry of vision and the role of photochemical reactions in natural processes.

1. **Photochemistry** **(16 L)**

Photo rearrangements of cyclopentanone , cyclohexanone, dienones, β-r unsaturated ketones, Aza-Di-**π**–Methane rearrangement, Di-**π**–Methane rearrangement, rearrangements in aromatic compounds, photo reduction and photo oxidation , photo substitution reaction at sp^3 carbon having one hydrogen - Barton reaction.

Photochemistry in nature- chemistry of vision, Application of photochemical reactions in synthesis – Isocomene Ref. 1,2,3,4

2. **Free radicals:** **[16 L]**

Radical initiators, Characteristic s reactions,- Free radical substitution ,addition to multiple bonds, free radical halogenations - chlorinationand bromination-NBS ,autoxidation, Thermal decomposition of hydroperoxides, Radicals in synthesis: Hunsdiecker reaction,Barton Nitrite Photolysis reaction ,Barton Decarboxylation, Inter and intramolecular C-C bond formation via mercuric hydride ,tin hydride, , Oxidative coupling. C-C bond formation in aromatics, SNAr reactions-Sandmeyer reaction Ref. 1, 3, 6

3. **Pericyclic reactions** **[16 L]**

Recapitulation of Molecular Orbitals, their symmetry properties, Woodward –Hoffmann's Conservation of orbital symmetry property rule.

Cycloaddition reactions, Chelotropic reactions, Sigmatropic reactions, and 1,3-dipolar additions, Analysis by correlation diagrams, Mobius Huckel theory and ATS concept. Application of pericyclic reactions: Ene reaction, Sommelet Hauser rearrangement, Claisen and Cope rearrangements, fluxional molecules, synthesis of Endiandric acid.

Ref.1, 3,5, 7,10-14

References:

1. Advanced Organic Chemistry, Part A – F. A. Carey and R. J. Sundberg, 5th Ed.Springer(2007)
2. Excitedstatesin Organic Chemistry-J.A.Barltrop andJ.D.Coyle, JohnWiley&sons
3. Photochemistryand Pericyclicreactions-Jagdamba Singh, Jaya Singh 3rdEd.
4. Organicphotochemistry:Avisualapproach-JanKopecky,VCHpublishers (1992).
5. Conservation of orbital symmetry – R. B. Woodward and R. Hoffmann; VerlagChemie,Academic press(1971).
6. RadicalsinOrganicSynthesisB.Giese,Pergamonpress(1986)
7. Orbital Symmetry : A problem solving approach- R. E. Lehr and A. P.Marchand;Academic (1972)
8. Classicsintotal synthesis-K. C.Nicolaouand E.J. Sorensen;VHC(1996)

9. P.A. Wenderand J. J. Howbert*J. Am.Chem. Soc.* **1981**,*103*, 688-690.
10. Organicreactionsandorbitalsymmetry,2ndEd.T. L.GilchristandR.C.Storr
11. Organic Chemistry–J.Clayden,N. Greeves,S.WarrenandP. Wothers
12. Pericyclicreactions:Atextbook–S.Sankararaman
13. Pericyclicreactions-Gilland Willis
14. Frontierorbitals andorganicchemicalreactions-Ian Fleming,John Wiley& sons7

Choice Based Credit System Syllabus
(2022 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III) **Subject**:Organic Chemistry
Course: Photochemistry, Free radicals and Pericyclic Reactions **Course Code**: PSCHO-234
Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	0	0	3	0	0	0
CO2	3	3	0	0	0	3	0	0	0
CO3	0	3	0	2	0	0	0	0	0
CO4	3	3	0	0	0	3	0	0	0
CO5	3	0	0	2	0	2	0	0	0
CO6	3	3	0	0	2	3	0	0	2
CO7	0	0	0	2	2	3	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):
CO1. Understand the principles and mechanisms of photochemical reactions, including photo rearrangements, photo reduction, and photo oxidation.
CO2. Apply the concepts of photochemistry to analyze and predict the outcomes of photo substitution reactions, such as the Barton reaction.
CO4. Describe the characteristics and reactions of free radicals, including free radical substitution and addition to multiple bonds.
CO5. Apply free radicals in various synthetic reactions, such as the Hunsdiecker reaction and
Barton Nitrite Photolysis reaction.
CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.

PO2 (Critical Thinking and Problem Solving):
CO2, CO3, CO4, and CO6 exhibit a strong alignment, indicating a focus on developing critical thinking skills in the context of photochemical reactions and their applications.
CO2. Apply the concepts of photochemistry to analyze and predict the outcomes of photo substitution reactions, such as the Barton reaction.
CO3. Utilize photochemical reactions in synthesis, specifically the Isocomene synthesis.
CO4. Describe the characteristics and reactions of free radicals, including free radical

substitution and addition to multiple bonds.
CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.

PO4 (Research-related Skills and Scientific Temper):
CO3, CO5, and CO7 show a moderate alignment, indicating a focus on research-related skills, especially in utilizing photochemical reactions in synthesis and explaining the chemistry of vision.
CO3. Utilize photochemical reactions in synthesis, specifically the Isocomene synthesis.
CO5. Apply free radicals in various synthetic reactions, such as the Hunsdiecker reaction and
Barton Nitrite Photolysis reaction.
CO7. Explain the chemistry of vision and the role of photochemical reactions in natural processes.

PO5 (Trans-disciplinary Knowledge):
CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.
CO7. Explain the chemistry of vision and the role of photochemical reactions in natural processes.

PO6 (Personal and Professional Competence):
CO1. Understand the principles and mechanisms of photochemical reactions, including photo rearrangements, photo reduction, and photo oxidation.
CO2. Apply the concepts of photochemistry to analyze and predict the outcomes of photo substitution reactions, such as the Barton reaction.
CO4. Describe the characteristics and reactions of free radicals, including free radical substitution and addition to multiple bonds.
CO5. Apply free radicals in various synthetic reactions, such as the Hunsdiecker reaction and
Barton Nitrite Photolysis reaction.
CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.
CO7. Explain the chemistry of vision and the role of photochemical reactions in natural processes.

PO9 (Self-directed and Life-long Learning):
CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.

Practical course I

PSCHO-235:Single stage preparations

[4Credits]

Course Objective:

1) Develop proficiency in performing organic synthesis and purification techniques, including the use of appropriate laboratory equipment and methods for the synthesis and purification
2) Acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds, such as cyclization reactions, functional group transformations.
3) Gain knowledge about the principles and mechanisms of reduction reactions
4) Understand the principles and mechanisms of formylation reactions and gain practical experience through formylation experiments,
5) Develop an understanding of the fundamental principles and concepts of the isolation of natural products, including extraction techniques, purification methods,
6) Develop practical skills in handling and manipulating organic compounds, including proper techniques for weighing, measuring, and transferring reagents, as well as safe handling and disposal of hazardous materials
7) Develop practical skills in handling and synthesizing organic compounds

Course Outcomes : On completion of the course, the student should be able to;

CO1. Students will gain proficiency in performing organic synthesis and purification techniques.

CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.

CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.

CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.

CO5. Enhancing communication skills by effectively documenting experimental procedures and results.

CO6. Understanding the fundamental principles and concepts of isolation of natural products.

CO7. Developing practical skills in handling and manipulating organic compounds.

At least nine single stage and five isolation of Natural products and two quantitative analysis should be carried out. The preparation should be carried out on micro scale.

A) Advance organic practical (any 9)

Synthesis, purification and characterization of:

1) 2-phenyl indole by Fischer indole synthesis
2) Benzyl alcohol and benzoic acid from benzaldehyde (Canninzaro reaction)
3) 2-chlorobenzoic acid from anthranillic acid (Sandmeyer reaction)
4) Cyclohexanol from cyclohexanone ($NaBH_4$ reduction)
5) 4-Nitro Benzonitrile from 4-Nitrobenzaldehyde
6) Imidazole from orthophenylene diamine
7) Osazone from glucose
8) Schiff base synthesis from substituted benzaldehyde
9) 4-amino benzoic acid from 4-Nitro benzoic acid
10) Synthesis of chalcone from substituted benzaldehyde
11) 2- amino 4-phenyl thiazole from acetophenone and thiourea
12) O-Benzoyloxyacetophenone from O-hydroxyacetophenone (Flavone)

B) Isolation of Natural products (Any2)

1) Piperine from pepper
2) Eugenol from clove
3) Cinnmaldehyde from cinnamon

Choice Based Credit System Syllabus
(2022 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III) **Subject**:Organic Chemistry
Course: Single stage preparations **Course Code**: PSCHO-235
Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	2	0	3	0	0	2
CO2	3	3	0	2	2	3	0	0	2
CO3	3	3	0	2	0	0	0	0	0
CO4	3	3	0	3	2	0	0	0	2
CO5	3	3	0	0	0	3	0	0	2
CO6	0	3	0	2	2	3	0	0	2
CO7	3	0	0	0	0	3	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):

CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.
CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
CO7. Developing practical skills in handling and manipulating organic compounds.

PO2 (Critical Thinking and Problem Solving):

CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.
CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
CO6. Understanding the fundamental principles and concepts of isolation of natural products.

PO4 (Research-related Skills and Scientific Temper):

CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.
CO6. Understanding the fundamental principles and concepts of isolation of natural products.

PO5 (Trans-disciplinary Knowledge):
CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
CO6. Understanding the fundamental principles and concepts of isolation of natural products.

PO6 (Personal and Professional Competence):
CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
CO6. Understanding the fundamental principles and concepts of isolation of natural products.
CO7. Developing practical skills in handling and manipulating organic compounds.

PO9 (Self-directed and Life-long Learning):
CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
CO6. Understanding the fundamental principles and concepts of isolation of natural products.

Practical course II

PSCHO-236: Double and multiple stage preparations

[4credits]

Course Objective:

1) To teach students to break down complex target molecules into simpler, readily available starting materials using retrosynthetic principles. This involves identifying key functional groups and strategic disconnections.
2) To familiarize students with a wide range of reactions and techniques for the conversion of one functional group into another.
3) Understanding reaction mechanisms, regioselectivity, and stereoselectivity.
4) To develop students' skills in designing multi-step synthetic routes based on the selection of appropriate reactions and reagents.
5) To introduce students to practical laboratory techniques commonly used in multi-step organic synthesis, including purification methods, separation techniques, and characterization techniques (such as spectroscopy).
6) To enhance students' problem-solving skills and critical thinking abilities by providing them with opportunities to analyze complex synthetic problems and propose efficient solutions.
7) To emphasize the importance of safety protocols and ethical considerations in the practice of organic chemistry, particularly in multi-step synthesis involving potentially hazardous reagents or reactions.

Course Outcomes : On completion of the course, the student should be able to;

CO1. Understanding the principles and mechanisms of nitration, sulphonation, oxidation, reduction, and hydrolysis reactions in double stage preparation.

CO2. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.

CO3. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.

CO4. Gaining proficiency in performing laboratory techniques and procedures involved in the double stage preparation.

CO5. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.

CO6. Enhancing problem-solving abilities by troubleshooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.

CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

A) Double stage preparation (any 6)

1) Benzaldehyde to benzalacetophenone to epoxide
2) Cyclohexanone to phenylhydrazone to 1,2,3,4-tetrahydrocarbazole
3) Phthalic anhydride to phthalimide to anthranilicacid
4) Acetanilide to 4-nitroacetanilide to 4-nitroaniline
5) Benzyl cyanide to 4-nitro benzyl cyanide to 4-nitro phenyl acetic acid
6) Nitrobenzene to m-dinitrobanzene to m-nitro aniline
7) Benzanilide from benzophenone by Beckmann rearrangement.
8) P-nitro actanilide to p-nitroaniline to p-iodonitrobenzene
9) Phthalimide to n-benzyl Phthalimide to benzylamine
10) Preparation of P-amino benzoic acid
11) acetophenone to 2- amino 4-phenyl thiazole to substituted Schiff base
12) Preaparation of N-Bromosuccinamide
13) Structure elucidation by using given spectral data.

Choice Based Credit System Syllabus
(2022 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III) **Subject**:Organic Chemistry
Course: Double and multiple stage preparations **Course Code**: PSCHO-236
Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**
CO1	3	0	0	0	0	3	0	0	0
CO2	3	3	0	0	0	3	0	0	0
CO3	3	3	0	2	0	0	0	0	0
CO4	3	0	0	0	2	0	0	0	0
CO5	3	0	0	3	0	3	0	0	0
CO6	3	3	0	2	0	3	0	0	1
CO7	0	3	0	2	2	3	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):
CO1. Understanding the principles and mechanisms of nitration, sulphonation, oxidation, reduction, and hydrolysis reactions in double stage preparation.
CO2. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.
CO3. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.
CO4. Gaining proficiency in performing laboratory techniques and procedures involved in the double stage preparation.
CO5. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.

PO2 (Critical Thinking and Problem Solving):
CO2. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.
CO3. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.
CO6. Enhancing problem-solving abilities by troubleshooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.
CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO4 (Research-related Skills and Scientific Temper):
CO3. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.
CO5. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.
CO6. Enhancing problem-solving abilities by troubleshooting and optimizing reaction

conditions to improve the yield and selectivity of the desired compounds.
CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO5 (Trans-disciplinary Knowledge):
CO4. Gaining proficiency in performing laboratory techniques and procedures involved in the double stage preparation.
CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO6 (Personal and Professional Competence):
CO1. Understanding the principles and mechanisms of nitration, sulphonation, oxidation, reduction, and hydrolysis reactions in double stage preparation.
CO2. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.
CO5. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.
CO6. Enhancing problem-solving abilities by troubleshooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.
CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO9 (Self-directed and Life-long Learning):
CO6. Enhancing problem-solving abilities by trouble shooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.